Final Report for AOARD Grant FA2386-11-1-4065 AOARD Grant 114065 "Pushing the material limits in high κ dielectrics on high carrier mobility semiconductors for science/technology beyond Si CMOS and more"

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Abstract: Our research activities during the last eight years from 2006 to 2013, with the grant supports from Nano National programs, NSC, Taiwan and AOARD, have been pushing the material limits of III-V InGaAs and GaN metal-oxide-semiconductor (MOS) systems using high κ dielectrics. In the third year of the funding, with the capabilities of atomic-scale probing and manipulating the high k oxides/semiconductors interfaces, we have established the correlations between electronic structures and electrical properties essential to understand the Fermi level pinning/unpinning mechanism of the interfaces between metal/oxide and oxide/semiconductor. we have successfully continuously kept our world-leading expertise of high- κ dielectric growth on InGaAs by achieving world record drain current of 1.8 mA/μm, transconductance of 0.80 mS/μm, and low sub-thresholds in a self-aligned inversion-channel InGaAs metal-oxide-semiconductor field-effect- transistor of 1 μm gate length. *In-situ* ultrahigh vacuum deposited Y₂O₃ and HfO₂ and atomic-layer-deposited (ALD) Al₂O₃ and HfO₂ 2-3 mono-layers thick on freshly grown In_{0.53}Ga_{0.47}As, with an Al₂O₃ cap, were employed as a gate dielectric.

Furthermore, high quality nm-thick Gd_2O_3 and Y_2O_3 (rare-earth oxide, R_2O_3) films have been epitaxially grown on GaN (0001) substrate by molecular beam epitaxy (MBE). The R_2O_3 epilayers exhibit remarkable thermal stability at $1100^{\circ}C$, uniformity, and highly structural perfection. Structural investigation was carried out by *in-situ* reflection high energy electron diffraction (RHEED) and *ex-situ* X-ray diffraction (XRD) with synchrotron radiation. In the initial stage of epitaxial growth, the R_2O_3 layers have a hexagonal phase with the epitaxial relationship of R_2O_3 (0001)H[11-20]H/GaN(0001)H[11-20]H. With the increase in R_2O_3 film thickness, the structure of the R_2O_3 films changes from single domain hexagonal phase to monoclinic phase with six different rotational domains, following the R_2O_3 (-201)H[020]H/GaN(0001)H[11-20]H orientational relationship. The structural details and fingerprints of hexagonal and monoclinic phase Gd_2O_3 films have also been examined by using electron energy loss spectroscopy (EELS). Approximate 3-4 nm is the critical thickness for the structural phase transition depending on the composing rare earth element.

Introduction: Hetero-epitaxy between two dissimilar materials has been the key for producing artificial structured materials, the building blocks for new sciences, novel devices and advanced technologies. Particularly, the epitaxial growth among oxides and semiconductors has always been scientifically intriguing and technologically relevant. One notable example is the successful growth of single crystal GaN on sapphire and Si(111), which has led to the recent commercialization of solid state lighting and high power devices. The growth of single crystal Gd_2O_3 on $GaAs(001)^6$ is another example, leading to the first

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14. ABSTRACT

Our research activities during the last eight years from 2006 to 2013, with the grant supports from Nano National programs, NSC, Taiwan and AOARD, have been pushing the material limits of III-V InGaAs and GaN metal-oxide-semiconductor (MOS) systems using high dielectrics. In the third year of the funding, with the capabilities of atomic-scale probing and manipulating the high k oxides/semiconductors interfaces, we have established the correlations between electronic structures and electrical properties essential to understand the Fermi level pinning/unpinning mechanism of the interfaces between metal/oxide and oxide/semiconductor. we have successfully continuously kept our world-leading expertise of high-dielectric growth on InGaAs by achieving world record drain current of 1.8 mA/m, transconductance of 0.80 mS/m, and low sub-thresholds in a self-aligned inversion-channel InGaAs metal-oxide-semiconductor field-effect- transistor of 1 m gate length. In-situ ultra-high vacuum deposited Y2O3 and HfO2 and atomic-layer-deposited (ALD) Al2O3 and HfO2 2-3 mono-layers thick on freshly grown In0.53Ga0.47As, with an Al2O3 cap, were employed as a gate dielectric.

15. SUBJECT TERMS

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demonstration of inversion-channel GaAs metal-oxide-semiconductor field-effect-transistors (MOSFETs),⁹ timely for the ultimate complementary MOS (CMOS) technology.^{10,11}

 Gd_2O_3 and Y_2O_3 of cubic phase were found to grow epitaxially on Si, Ge, and GaAs. The lattice constants of cubic Gd_2O_3 and Y_2O_3 are 10.8 and 10.6 Å, respectively, which are approximately twice those of GaAs, Si, and Ge, being 5.65, 5.43, and 5.65 Å, respectively. The oxides deposited on Si(111) exhibit the same (111) surface normal. The oxides deposited on the (001) oriented GaAs, Si, and Ge^{14} , however, have (011) parallel with the (001) normal of the semiconductors. The in-plane lattice spacing of the oxide (011) does not match well with those of GaAs, Si, Si, Si, Si, Si, and Ge, indicating the bond arrangement and the energy consideration at the oxide/semiconductor interfaces are more critical than the crystalline symmetry.

Besides the epitaxial growth, an effective passivation of high dielectrics on semiconductor has been intensively studied as higher device performance demands smaller device sizes and thinner gate dielectrics. GaN and its related compounds, which have been used for high-temperature high-power RF electronics because of the large critical breakdown fields and high saturation velocities, 18 are now being considered for the post Si CMOS. Recently, GaN MOSFETs have been demonstrated using MgO, 19,20 Al₂O₃,21 HfO₂,22 and Ga₂O₃(Gd₂O₃)²³ as the gate dielectrics. For pushing the GaN MOS technology, the equivalent oxide thickness (EOT) of the gate dielectric is required to be much less than 1 nm. 11 Therefore, the dielectric constant of the gate dielectric has to be enhanced. Moreover, self-aligned inversion-channel GaN MOSFETs may require the gate dielectric to be of single crystal as amorphous films tend to form poly-crystalline resulting from the high temperature source/drain (S/D) dopant activation process; the gate dielectric needs to sustain rapid thermal annealing (RTA) process up to 1100°C for at least 5 mins.²⁴ High-quality hexagonal phase Gd₂O₃ with good crystallinity has been successfully deposited on c-plane GaN and shows excellent electrical properties. 25,26 More recently, the monoclinic Gd₂O₃ and Y₂O₃ layers consisting of six different rotational domains on GaN have also been reported.²⁷⁻²⁹ The monoclinic phase of rare earth oxides is not energetically favorable under ambient condition. The presence of these non-ambient phases is attributed to epitaxial stabilization.

In this work, we have systematically scaled down the thickness of the molecular beam epitaxy (MBE) deposited Gd_2O_3 and Y_2O_3 on GaN from 10-20 nm to 1-2 nm. With decreasing layer thickness to 2-4 nm, the structure of the rare-earth oxides changes from monoclinic phase to hexagonal phase. There are great similarities on the structural properties between Gd_2O_3 and Y_2O_3 . The discussion will, therefore, focus on Gd_2O_3 . The structural characterizations were performed by high resolution X-ray diffraction (HRXRD) with synchrotron radiation.

Results and Discussion: The RHEED pattern of the starting GaN surface was a streaky reconstructed (2 \times 2) along GaN <11 $\bar{2}$ 0> and <10 $\bar{1}$ 0>, respectively. With the Gd₂O₃ thickness larger than 0.8 nm, the patterns turned to a streaky (1 \times 1) and with the thickness increasing to >5 nm, a reconstructed (3 \times 2) appeared, which remained unvaried all the way to 20 nm;²⁸ The patters remained streaky during the growth, indicating two-dimensional growth. From the systematic X-ray diffraction study as will be discussed later, the initial growth of Gd₂O₃ has yielded a hexagonal phase with surface normal (0001) and in-plane axes of Gd₂O₃ being parallel to the corresponding axes of GaN.

The X-ray diffraction scans along the surface normal of the Gd_2O_3 samples with different oxide thickness are shown in Fig. 1. The intense sharp peaks of GaN (0002), GaN (0004) and sapphire (0006) reflections are, respectively, centered at 2.0, 4.0, and 2.395 rlu_{GaN} , the reciprocal lattice unit of GaN along its c-axis with 1 $rlu_{GaN} = 2\pi/c_{GaN} = 1.212 \text{ Å}^{-1}$. The oxide peaks are those with the periodic thickness fringes, which are caused by the interference between the X-rays reflected by the top surface and buried interface. The presence of the

pronounced fringes revealed a very smooth surface/interface and good crystalline quality of the Gd₂O₃ epitaxial layer on GaN.

For Gd_2O_3 films with thickness of 1.5, 2.2, and 3.2 nm, aside from the main substrate signals, two broad oxide peaks were centered at ~1.73 and ~3.44 rlu_{GaN}. The broadness came from the short structural coherence length limited by the small layer thickness. The interplanar spacing corresponding to these peaks was close to that of monoclinic phase $(\bar{4}02)_M$, $(\bar{8}04)_M$ and hexagonal phase $(0002)_H$, $(0004)_H$ planes; it would be very difficult to assign phases based on the observed reflections alone. However, for thicker Gd_2O_3 films of 4.3 and 10 nm, two additional peaks centered at ~0.87 and ~2.61 rlu_{GaN} were found. Based on JCPDS cards (No 42-1465), these latter two peaks correspond to $(\bar{2}01)_M$ and $(\bar{6}03)_M$ reflections, and no allowed reflection belonging to the hexagonal phase exists in the nearby region. The absence of these two peaks in the films less than ~4 nm thick, therefore, indicates that the thinner Gd_2O_3 films have a hexagonal structure. The two oxide peaks of the three thinnest oxide layers were then indexed as the $(0002)_H$ and $(0004)_H$ reflections of the H-Gd₂O₃. For oxide films with thickness above 4 nm, the broad peaks centered at 0.87, 1.75, 2.61, 3.48 and 4.35 rlu_{GaN} were indexed as $(\bar{2}01)_M$, $(\bar{4}02)_M$, $(\bar{6}03)_M$, $(\bar{8}04)_M$ and $(\bar{1}005)_M$ reflections of M-Gd₂O₃, respectively.

The scans along surface normal alone would not provide the off-normal crystallographic information, which is needed for accurately determining the symmetry of the oxide films and the alignment between the oxides and the substrates. Lateral radial scans were thus performed along the GaN in-plane $<11\bar{2}0>_{\rm H}$ direction, shown in Fig. 2. The measurements were performed in the grazing incidence diffraction geometry by keeping the surface normal almost perpendicular to the vertical scattering plane. For the Gd₂O₃ layers of thickness less than 4 nm, in addition to the narrow GaN $(11\overline{2}0)$ reflection centered at 1 rlu_{GaN}, the reciprocal lattice unit of GaN along the lateral direction with the magnitude of $4\pi/(\sqrt{3}a_{GaN}) = 2.274 \text{ Å}^{-1}$, a broad peak appears at 0.855 rlu_{GaN}. Both peaks exhibit 6-fold symmetry in azimuthal ϕ scans against the surface normal (not shown), revealing the hexagonal crystalline structure. The broad peak was indexed as the H-Gd₂O₃ $(11\bar{2}0)_{H}$ reflection, which is aligned with the GaN (1120) reflection. For the samples with Gd₂O₃ thickness greater than 4 nm, the oxide peak splits into two broad peaks, centered at 0.835 and 0.88 rlu_{GaN}, respectively. Even though their azimuthal scans also have 6 evenly spaced peaks, each peak further splits (not shown). The observed 6-fold symmetry and peak splitting can be accounted for by the coexistence of 6 rotational domains of M-Gd₂O₃ with $(\overline{2}01)_{M}$ normal and each domain has its $[020]_{M}$ axis aligned with one of the 6-fold symmetric GaN $<11\overline{2}0>$ direction.²⁸ The two peaks at 0.835 and 0.88 rlu_{GaN} in Fig. 2 are indexed as $(3\pm13)_{\rm M}$ and $(0\pm20)_{\rm M}$, respectively.

To further verify the crystalline structure of the hetero-epitaxial system, we performed reciprocal space mapping (RSM) around Gd_2O_3 $(1\,\bar{1}\,01)_H$ reflection in the GaN h-/ plane. A clean oval-shape peak was obtained from the thin layers with thickness less than 4 nm, as illustrated in Fig. 3(a), (b) and (c), indicating that H-Gd $_2O_3$ possesses only one domain. The reduction in the profile elongation along the / direction reflects the increase of vertical structural coherence length associated with the increasing layer thickness. As the thickness increases beyond 4 nm, the peak profile gradually evolves into a cluster of 4 peaks. According to the model of $(\bar{2}\,01)_M$ oriented M-Gd $_2O_3$ with six rotational domains, the four maxima in the RSM shown in Fig. 3(d), (e), and (f) are associated with the Gd $_2O_3$ $(\bar{4}0\bar{1})_M$, $(\bar{3}\pm10)_M$, $(\bar{1}\pm12)_M$, and $(003)_M$ reflections, in the order of increasing /value, belonging to six different rotational domains. The evolution of the Gd $_2O_3$ reflection from a single maximum to four peaks in the RSM shown in Fig. 3 as the oxide thickness increases attest the structural transition from the hexagonal to the monoclinic phase and the critical thickness is

approximately 4 nm.

By fitting the angular positions of many reflections, we derived the lattice parameters of the hexagonal phase to be a = b = 3.75 Å and c = 5.94 Å, similar to the results of ab initio energetic calculations based on the density functional theory (DFT) and projector augmented wave (PAW) pseudo-potentials method. Similarly, the monoclinic phase lattice constants are determined to be a = 13.965 Å, b = 3.595 Å, c = 8.787 Å, and β = 101.34°. According to the phase diagram, bulk Gd₂O₃ exists in three polymorphic forms: cubic ($Ia\bar{3}$), monoclinic (C2/m), and hexagonal ($P\bar{3}m1$) at temperature below ~2,500K and the cubic phase with the bixbyite structure is the one stable at the ambient condition. The hexagonal phase only exists at high pressure or high temperature. It is thus difficult to accurately determine the strain state of the hexagonal phase oxide layers because of the lack of ambient condition data to compare with. Nevertheless, the lattice parameters of H-Gd₂O₃ layer remained practically unchanged and their values are close to the theoretic prediction, implying the lattice is nearly fully relaxed.

Summary: Gd_2O_3 and Y_2O_3 epi-layers on GaN (0001) have the hexagonal phase with their thickness less than a critical value t_c (3~4 nm), as stabilized by epitaxy. The hexagonal to monoclinic phase transition occurs as thickness exceeds t_c . The stabilization of the hexagonal phase at a few nm-thick with high thermal stability, a high dielectric constant, and a low interfacial density of states strongly favors the application of sing le crystal Gd_2O_3 and Y_2O_3 as gate dielectrics for advanced GaN MOS devices with low EOT.

References:

- 1. National Research Council, In *Condensed-Matter Physics*, The National Academies Press: Washington, D.C., **1986**.
- 2. Kwo, J.; Hong, M.; Nakahara, S. Appl. Phys. Lett. 1986, 49, 319-321.
- 3. Nakamura, S.; Mukai, T.; Senoh, M. Appl. Phys. Lett. 1994, 64, 1687-1689.
- 4. Egawa, T.; Zhang, B.; Ishikawa, H. IEEE Electron Device Lett. 2005, 26, 169-171.
- 5. Iwakami, S.; Machida, O.; Yanagihara, M.; Ehara, T.; Kaneko, N.; Goto, H.; Iwabuchi, A. *Jpn. J. Appl. Phys.* **2007**, *46*, L587-L589.
- Hong, M.; Kwo, J.; Kortan, A. R.; Mannaerts, J. P.; Sergent, A. M. Science 1999, 283, 1897-1900.
- 7. Nozaki, T.; Hirohata, A.; Tezuka, N.; Sugimoto, S.; Inomata, K. *Appl. Phys. Lett.***2005**, *86*, 082501.
- 8. Lin, B. H.; Liu, W. R.; Yang, S.; Kuo, C. C.; Hsu, C.-H.; Hsieh, W. F.; Lee, W. C.; Lee, Y. J.; Hong, M.; Kwo, J. C*ryst. Growth Des.* **2011**, *11*, 2846-2851.
- 9. Ren, F.; Hong M. W.; Hobson W. S.; Kuo, J. M.; Lothian, J. R.; Mannaerts, J. P.; Kuo, J.; Chen, Y. K.; Cho, A. Y. *IEEE International Electron Devices Meeting*, **1996**, 943-945.
- 10. Kuhn, K. J. IEEE T. Electron Dev. 2012, 59, 1813-1828.
- 11. International Technology Roadmap for Semiconductor 2011 edition. Homepage, http://www.itrs.net/Links/2011ITRS/Home2011.htm
- 12. Lin, T. D.; Hang, M. C.; Hsu, C. H.; Kwo, J.; Hong, M. *J. Cryst. Growth* **2007**, *301-302*, 386–389.
- 13. Kwo, J.; Hong, M.; Kortan, A. R.; Queeney, K. T.; Chabal, Y. J.; Mannaerts, J. P.; Boone, T.; Krajewski, J. J.; Sergent, A. M.; Rosamilia, J. M. *Appl. Phys. Lett.* **2000**, *77*, 130-132.
- 14. Molle, A.; Wiemer, C.; Bhuiyan, M. N. K.; Tallarida, G.; Fanciulli, M.; Pavia, G. *Appl. Phys. Lett.***2007**, *90*, 193511.
- 15. Sowwan, M; Yacoby, Y.; Pitney, J.; MacHarrie, R.; Hong, M.; Cross, J.; Walko, D. A.; Clarke, R.; Pindak, R.; Stern, E. A. *Phys. Rev. B* **2002**, *66*, 205311.
- 16. Kwo, J.; Hong, M.; Kortan, A. R.; Queeney, K. L.; Chabal, Y. J.; Opila, R. L.; Muller, D. A.; Chu, S. N. G.; Sapjeta, B. J.; Lay, T. S.; Mannaerts, J. P.; Boone, T.; Krautter, H. W.; Krajewski, J. J.; Sergnt, A. M.; Rosamilia, J. M. *J. Appl. Phys.* **2001**, *89*, 3920-3927.

- 17. Molle, A.; Perego, M.; Bhuiyan, Md. N. K.; Wiemer, C.; Tallarida, G.; Franciulli, M. *J. Appl. Phys.* **2007**, *102*, 034513.
- 18. Morkoc, H.; Strite, S.; Gao, G. B.; Lin, M. E.; Sverdlov, B.; Burns, M. *J. Appl. Phys.* **1994**, *76*, 1363-1398.
- 19. Irokawa, Y.; Nakano, Y.; Ishiko, M.; Kachi, T.; Kim, J.; Ren, F.; Gila, B. P.; Onstine, A. H.; Abernathy, C. R.; Pearton, S. J.; Pan, C.-C.; Chen, G.-T.; Chyi, J.-I. *Appl. Phys. Lett.***2004**, *84*, 2919-2921.
- 20. Lee, K. T.; Huang, C. F.; Gong, J.; Lee, C. T. *IEEE Electron Device Lett.***2011**, *32*, 306-308.
- 21. Chang, Y. C.; Chang, W. H.; Chiu, H. C.; Tung, L. T.; Lee, C. H.; Shiu, K. H.; Hong, M.; Kwo, J.; Hong, J. M.; Tsai, C. C. *Appl. Phys. Lett.* **2008**, *93*, 053504.
- 22. Chang, Y. C.; Chang, W. H.; Chang, Y. H.; Kwo, J.; Lin, Y. S.; Hsu, S. H.; Hong, J. M.; Tsai, C. C.; Hong, M. *Microelectron. Eng.* **2010**, *87*, 2042-2045.
- 23. Ren, F.; Hong, M.; Chu, S. N. G.; Marcus, M. A.; Schurman, M. J.; Baca, A.; Pearton, S. J.; Abernathy, C. R. *Appl. Phys. Lett.* **1998**, *73*, 3893-3895.
- 24. Matocha, K.; Chow, T. P.; Gutmann, R. J. IEEE T. Electron Dev. 2005, 52, 6-10.
- 25. Hong, M.; Kwo, J.; Chu, S.N.G.; Mannaerts, J. P.; Kortan, A. R.; Ng, H. M.; Cho, A. Y.; Anselm, K. A.; Lee, C. M.; Chyi, J. I. *J. Vac. Sci. Technol. B* **2002**, *20*, 1274-1277.
- 26. Chang, W. H.; Lee, C. H.; Chang, Y. C.; Chang, P.; Huang, M. L.; Lee, Y. J.; Hsu, C. H.; Hong, J. M.; Tsai, C. C.; Kwo, J.; Hong, M. *Adv. Mater.* **2009**, *21*, 4970-4974.
- 27. Chang, W. H.; Lee, C. H.; Chang, P.; Chang, Y. C.; Lee, Y. J.; Kwo, J.; Tsai, C. C.; Hong, J. M.; Hsu, C. -H.; Hong, M. *J. Cryst. Growth* **2009**, *311*, 2183-2186.
- 28. Chang, W. H.; Chang, P.; Lai, T. Y.; Lee, Y. J.; Kwo, J.; Hsu, C. -H.; Hong, M. Cryst. *Growth Des.* **2010**, *10*, 5117-5122.
- 29. Chang, W. H.; Chang, P.; Lee, W. C.; Lai, T. Y.; Kwo, J.; Hsu, C. -H.; Hong, J. M.; Hong, M. *J. Cryst. Growth* **2011**, *323*, 107-110.
- 30. JCPDS cards (No 42-1465)
- 31. Wu, B.; Zinkevich, M.; Aldinger, F.; Wen, D.; Chen, L. *J. Solid State Chem.* **2007**, *180*, 3280-3287.
- 32. Zinkevich, M. *Prog. Mater. Sci.* **2007**, *52*, 597-647.
- 33. Warshaw, I.; Roy, R. J. Phys. Chem. 1961, 65, 2048-2051.
- 34. Sato, S.; Takahashi, R.; Kobune, M.; Gotoh, H. Appl. Catal. A-Gen. 2009, 356, 57-63.

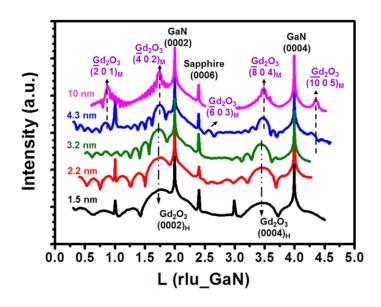


Fig. 1: XRD longitudinal scans along surface normal of samples with different Gd_2O_3 layer thickness.

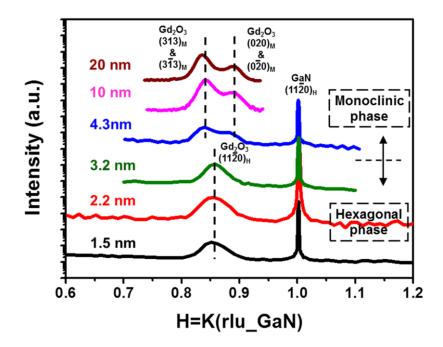


Fig. 2: Intensity distributions of in-plane radial scans along GaN $[11\bar{2}0]_H$ direction for Gd₂O₃ samples with thickness from 1.5 to 20 nm.

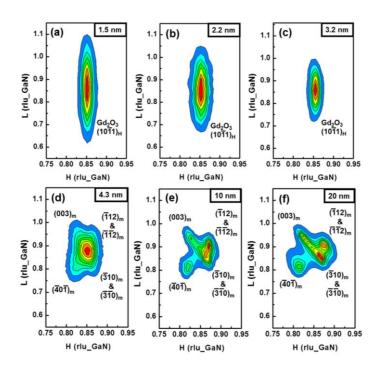


Fig. 3: The 2D reciprocal space maps in the GaN h-/plane near the Gd_2O_3 ($10\bar{1}1$) $_H$ reflection for the samples with a (a) 1.5 nm, (b) 2.2 nm, (c) 3.2 nm, (d) 4.3 nm, (e) 10 nm, and (f) 20 nm thick Gd_2O_3 epi-layer.

List of Publications:

Publications (SCI)

- "Metal Oxide Semiconductor Device Studies of Molecular-Beam-Deposited Al₂O₃/InP Heterostructures with Various Surface Orientations (001), (110), and (111)", L.-K. Chu, C. Merckling, J. Dekoster, J. R. Kwo, M. Hong, M. Caymax, and M. Heyns, Applied Physics Express 5, 061202 DOI: 10.1143/APEX.5.061202 (2012).
- 2. "Growth mechanism of atomic layer deposited Al2O3 on GaAs(001)-4x6 surface with trimethylaluminum and water as precursors", M. L. Huang, Y. H. Chang, T. D. Lin, S. Y. Lin, Y. T. Liu, T. W. Pi, M. Hong, and J. Kwo, Appl. Phys. Lett. 101, 212101 (2012) doi: 10.1063/1.4767129.
- 3. "Effective Passivation of In_{0.2}Ga_{0.8}As by HfO₂ Surpassing Al₂O₃ via *in-situ* Atomic Layer Deposition", Y. H. Chang, C. A. Lin, Y. T. Liu, T. H. Chiang, H. Y. Lin, M. L. Huang, T. D. Lin, T. W. Pi, J. Kwo, and M. Hong, Appl. Phys. Lett. 101, 172104 (2012).
- 4. "Phase transformation of molecular beam epitaxy-grown nanometer thick Gd_2O_3 and Y_2O_3 on GaN'', W. H. Chang, S. Y. Wu, C. H. Lee, T. Y. Lai, Y. J. Lee, P. Chang, C. H. Hsu, T. S. Huang, J. R. Kwo, and M. Hong, ACS Applied Materials & Interfaces 5, 1436 (2013).
- 5. "Inversion-channel GaAs(100) metal-oxide-semiconductor field-effect-transistors using molecular beam deposited Al_2O_3 as a gate dielectric on different reconstructed surfaces", Y. C. Chang, W. H. Chang, C. Merckling, J. Kwo, and M. Hong, Appl. Phys. Lett. 102, 093506 (2013).
- 6. "Atom-to-atom interactions for atomic layer deposition of trimethylaluminum on Ga-rich GaAs(001)-4x6 and As-rich GaAs(001)-2x4 surfaces: A synchrotron-radiation photoemission study", T.-W. Pi, H.-Y. Lin, Y.-T. Liu, T.-D. Lin, G. K. Wertheim, J. Kwo and M. Hong, Nanoscale Research Letters 8, 169 (2013).
- 7. "Interfacial electronic structure of trimethyl-aluminum and water on an In_{0.20}Ga_{0.80}As(001)-4x2 surface: A high-resolution core-level photoemission study", T. W. Pi (皮敦文)1, H. Y. Lin (林孝于) T. H. Chiang (江宗鴻), Y. T. Liu (劉雅婷), G. K. Wertheim, J. Kwo (郭瑞年), and M. Hong (洪銘輝), J. Appl. Phys. 113, 203703 (2013).
- 8. "Surface atoms core-level shifts in single crystal GaAs surfaces: Interactions with trimethylaluminum and water prepared by atomic layer deposition", T.W. Pi, H.Y. Lin, T.H. Chiang, Y.T. Liu, Y.C. Chang, T.D. Lin, G.K. Wertheim, ,J. Kwo, and M. Hong, Applied Surface Science 284, 601-610 (2013).
- "Surface Passivation of GaSb(100) Using Molecular Beam Epitaxy of Y₂O₃ and Atomic Layer Deposition of Al₂O₃: A Comparative Study", R.-L. Chu, W.-J. Hsueh, T.-H. Chiang, W.-C. Lee, H.-Y. Lin, T.-D. Lin, G. J. Brown, J.-I. Chyi, T.-S. Huang, T.-W. Pi, J. R. Kwo, and M. Hong, Appl. Phys. Express 6 121201 (2013).
- 10. "High-performance self-aligned inversion-channel In_{0.53}Ga_{0.47}As metal-oxide-semiconductor field-effect-transistors by *in-situ* atomic-layer-deposited HfO₂", T. D. Lin (林宗達), W. H. Chang (張文馨), R. L. Chu (朱瑞霖), Y. C. Chang (張耀中), Y. H. Chang (張宇行), M. Y. Lee (李美儀), P. F. Hong (洪鵬飛), Min-Cheng Chen (陳旻政), J. Kwo (郭瑞年), and M. Hong (洪鉛輝), Appl. Phys. Lett. **103**, 253509 (2013).

Conference presentations (Invited)

- "Realization of High k Gate Dielectrics on High Carrier Mobility Semiconductors Beyond Si CMOS", J. Kwo, M. Hong, W. W. Pai, Y. P. Chiu, T. W. Pi, and C. Merckling, the 17th International Conference on Molecular Beam Epitaxy (ICMBE), Nara, Japan, September 23 to 28, 2012.
- 2. "Realization of high performance InGaAs and Ge MOSFETs using MBE/ALD high-κ dielectrics", T. D. Lin, M. Hong, and J. Kwo, T. J. Watson Research Center IBM, October 2, 2012.
- 3. "Electrical defect analysis of InGaAs and Ge MOS devices passivated by ALD and MBE High-k dielectrics", C. A. Lin, M. Hong, and J. Kwo, T. J. Watson Research Center IBM, October 2, 2012.
- 4. "Overview of III-V Activities at National Taiwan University", M. Hong and J. Kwo, T. J. Watson Research Center IBM, October 2, 2012
- 5. "Electrical Analysis of In_xGa_{1-x}As MOS devices passivated by MBE and ALD High-k Dielectrics", C. A. Lin, M. Hong, and J. Kwo, 9th International Symposium on Advanced Gate Stack Technology, The Saratoga Hilton, Saratoga Springs, New York, USA, October 3–4, 2012.
- 6. "*In-situ* Deposited High κ Dielectrics for High Performance InGaAs MOS", T. D. Lin, M. Hong, and J. Kwo, 9th International Symposium on Advanced Gate Stack Technology, The Saratoga Hilton, Saratoga Springs, New York, USA, October 3–4, 2012.
- 7. "Atomic layer deposition and molecular beam epitaxy Pushing the material limit for CMOS scaling", M. Hong, J. Kwo, T. W. Pi, C. H. Hsu, W. W. Pai, and Y. P. Chiu, (plenary talk) The 1st International Conference on ALD Applications and the 2nd China ALD Conference, Fudan University, Shanghai, China, October 15-16, 2012.
- 8. "Native-oxides free high-k interfaces: A synchrotron radiation photoemission study", T.-W. Pi, T. D. Lin, H. Y. Lin, Y. T. Liu, Y. C. Chang, Y. H. Chang, G. K. Wertheim, J. Kwo, and M. Hong, (invited talk) The 1st International Conference on ALD Applications and the 2nd China ALD Conference, Fudan University, Shanghai, China, October 15-16, 2012.
- 9. "50 years of research/development of oxides on InGaAs leading to ultimate CMOS", M. Hong, Institute of Physics, Academia Sinica, Taipei, November 27, 2012.
- "Physics and Chemistry of the High k/InGaAs interface for High Carrier Mobility Channel MOSFET", J. Kwo, M. L. Huang, Y. C. Liu, C. A. Lin, W. C. Lee, Y. H. Chang, M. Hong, T. D. Lin, T. W. Pi, W. W. Pai, Y. M. Chang, 43rd IEEE Semiconductor Interface Specialist Conference (SISC), San Diego, CA, Dec. 5-8, 2012.
- 11. "Interfacial Properties of High k Gate Dielectrics on High Carrier Mobility Semiconductors", J. Kwo, Invited talk at Materials Research Society Spring Meeting, San Francisco, Ca, April 1-5, 2013.
- 12. "Native-oxides free high-k interfaces: A synchrotron radiation photoemission study", T.-W. Pi, T. D. Lin, H. Y. Lin, Y. T. Liu, Y. C. Chang, T. H. Chiang, G. K. Wertheim, J. Kwo, and M. Hong, invited talk at Materials Research Society Spring Meeting, San Francisco, Ca, April 1-5, 2013.
- 13. "Pushing the material limit and physics novelty in high k's/high carrier mobility

- semiconductors for *Ultimate CMOS"*, T. D. Lin, Y. C. Chang, M. Hong, J. Kwo, T. W. Pi, C. H. Hsu, W. W. Pai, and, Y. P. Chiu, Applied Materials, Hsinchu, Taiwan, May 22, 2013.
- 14. "Perfection of high k/InGaAs interface push for ultimate CMOS", 10th US Air Force Taiwan Nanoscience Workshop, New Sanno Hotel, Tokyo, Japan, Aug. 20-22, 2013.
- 15. "Realization of III-V MOSFETs using High k Gate Dielectrics on InGaAs Semiconductors", J. Kwo and M. Hong, the 2013 Asia-Pacific Radio Science Conference (AP-RASC'13), Howard International House, Taipei, Taiwan, September 3-7, 2013.
- 16. "Pushing the ultimate CMOS and more a physicist's role", Dept. Physics, National Chung Hsing University, Taichung, September 27, 2013.
- 17. "High k/III-V for ultimate CMOS from MBE to ALD passivation", T. D. Lin, J. Kwo, and M. Hong, 2013 IEEE Nanotechnology Materials and Devices Conference (IEEE NMDC), NCKU, Tainan, Taiwan, October 6-10, 2013.
- 18. "Synchrotron-radiation photoemission study of clean (In)GaAs surfaces and high-k interfaces", T. W. Pi, T. H. Chiang, Y. T. Liu, H. Y. Lin, Y. C. Chang, T. D. Lin, G. K. Wertheim, J. Kwo, and M. Hong, 2013 IEEE Nanotechnology Materials and Devices Conference (IEEE NMDC), NCKU, Tainan, Taiwan, October 6-10, 2013.

Conference presentations (Contributed)

- "Influence of initial GaAs reconstructed surfaces on the inversion-channel GaAs MOSFETs", Y. C. Chang, C. Merckling, W. H. Chang, J. Kwo, and M. Hong, 17th International MBE conference, Nara, Japan, Sep, 24-28, 2012.
- "Thermodynamic stability of MBE-HfO₂ on In_{0.53}Ga_{0.47}As", <u>T. D. Lin</u>, P. Chang, W. C. Lee, M. L. Huang, C. A. Lin, J. Kwo, and M. Hong, 17th International MBE conference, Nara, Japan, Sep, 24-28, 2012.
- 3. "Investigation of crystalline Gd₂O₃ phase transformation for advanced GaN MOS devices", W. H. Chang, S.Y. Wu, P. Chang, C. H. Lee, T.Y. Lai, Y. J. Lee, T. S. Huang, C. H. Hsu, J. Kwo, and M. Hong, 17th International MBE conference, Nara, Japan, Sep, 24-28, 2012.
- 4. "Investigation of MBE-grown In_{0.53}Ga_{0.47}As (001) 4x2 surface and in-situ ALD TEMA-Hf dosed surface by STM", Y. C. Liu, M. L. Huang, T. D. Lin, Y. T. Liu, W. C. Lee, W. W. Pai, M. Hong, and J. Kwo, 43rd IEEE Semiconductor Interface Specialist Conference, San Diego, CA, Dec. 5-8, 2012.
- "Electronic structure of (In)GaAs(001) surfaces and native oxide free high k interfaces", T.-W. Pi, T. D. Lin, H. Y. Lin, Y. T. Liu, Y. C. Chang, M. L. Huang, Y. H. Chang, G. K. Wertheim, J. Kwo, and M. Hong, 43rd IEEE Semiconductor Interface Specialist Conference, San Diego, CA, Dec. 5-8, 2012.
- 6. "Study of in-situ atomic-layer-deposited Al₂O₃ on GaAs (001) with different initial GaAs reconstructed surfaces", Y. T. Liu, H. Y. Lin, T. H. Chiang, Y. C. Chang, J. Kwo, and M. Hong, ROC Annual Physical Meeting, 中華民國物理學會年會, National Dong-Hwa University, Hua-Lien, Taiwan, Jan. 29-31, 2013.
- 7. "DLTS Measurement for low midgap interfacial trap density in In_{0.53}Ga_{0.47}As MOSCAPs by in-situ atomic-layer-deposited HfO₂ passivation", C. A. Lin (<u>林俊安</u>), M. C. Hsieh (謝孟謙), C. L. Tsai (蔡哲倫), Y. H. Chang(張宇行), T. D. Lin(林宗達), J. F. Chen(陳振芳), M. Hong (洪銘輝), and J. Kwo (郭瑞年), ROC Annual Physical Meeting, 中華民國物理學會年會,

- National Dong-Hwa University, Hua-Lien, Taiwan, Jan. 29-31, 2013.
- 8. "Investigation of MBE-grown In_{0.53}Ga_{0.47}As (001) 4x2 surface and in-situ ALD TEMA-Hf dosed surface by STM", Y. C. Liu (<u>劉有騏</u>), M. L. Huang (黃懋霖), T. D. Lin(林宗達), Y. T. Liu (劉雅婷), W. C. Lee (李威縉), H. Y. Lin (林孝于), W. W. Pai (白偉武), M. Hong (洪銘輝), and J. Kwo (郭瑞年), ROC Annual Physical Meeting, 中華民國物理學會年會, National Dong-Hwa University, Hua-Lien, Taiwan, Jan. 29-31, 2013.
- 9. "An improved interfacial passivation of employing molecule beam epitaxy grown Ge epilayer on Ge(100) substrate and *in-situ* high k dielectric deposition", R. L. Chu, W. C. Lee, Y. C. Liu, Y. C. Chang, H. Y. Lin, M. L. Huang, J. Kwo, and M. Hong, Symposium on Nano Device Technology, 國家奈米元件實驗室, National Nano Device Laboratories, Hsin-Chu, Taiwan, April 25-26, 2013
- 10. "Atomic layer deposited Al2O3 on Ga- and As-rich GaAs (100) reconstructed surfaces—electrical properties and interfacial chemical bonding", Y. T. Liu, W. H. Chang, Y. K. Su, Y. D. Wu, Y. C. Chang, J. Kwo, and M. Hong, Symposium on Nano Device Technology, 國家奈米實驗室, National Nano Device Laboratories, Hsin-Chu, Taiwan, April 25-26, 2013. SNDT
- 11. "UHV deposited rare earth oxides on GaAs (111)A growth, structural, electronic, and electrical properties", T. H. Chiang, S. Y. Wu, B. R. Chen, Y. K. Su, H. Y. Lin, C. A. Lin, J. Kwo, T. W. Pi, C.-H. Hsu, and M. Hong, Materials Research Society Spring Meeting, San Francisco, Ca, April 1-5, 2013.
- 12. "High k interfaces on single crystal (In)GaAs(001) surfaces", T.-W.Pi, T. D. Lin, Y. H. Chang, H. Y. Lin, Y. T. Liu, G. K. Wertheim, M. Hong, and J. Kwo, J. 38th International Conference on Vacuum Ultraviolet and X-ray Physics (VUVX2013), Hefei, Anhui, China, 12-19 July, 2013.
- 13. "Surface passivation of GaSb(100) using MBE-Y₂O₃ as gate dielectric", R. L. Chu, W. J. Hsueh, T. H. Chiang, W. C. Lee, H. Y. Lin, G. J. Brown, T. W. Pi, J. I. Chyi, J. Kwo, and M. Hong, 30th North American Molecular Beam Epitaxy Conference (NAMBE), Banff, Canada, Oct. 6-9, 2013.
- 14. "Perfecting high k/GaSb(100) interface using molecule beam epitaxy Y₂O₃", R. L. Chu, W. J. Hsueh, T. H. Chiang, W. C. Lee, H. Y. Lin, T. D. Lin, C. H. Fu, G. J. Brown, T. W. Pi, J. I. Chyi, J. Kwo, and M. Hong, 44th IEEE Semiconductor Interface Specialists Conference (SISC), Key Bridge Marriott Hotel, Arlington, VA, USA, December 5-7, 2013.
- 15. "Electronic structure of (In)GaAs surfaces and native-oxide free high k interfaces Synchrotron radiation photoemission studies", T.-W. Pi, T. D. Lin, T. H. Chiang, Y. T. Liu, Y. C. Chang, C. H. Wei, G. K. Wertheim, J. Kwo, and M. Hong, 44th IEEE Semiconductor Interface Specialists Conference (SISC), Key Bridge Marriott Hotel, Arlington, VA, USA, December 5-7, 2013.

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